Multiscale Large-Eddy Simulation

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The objective of this research was to improve existing turbulent flow simulations by more correctly modeling the energy transfer between very dissimilar scales. NASA will benefit from this research through improved simulation of fluid flows in and around aerospace vehicles and in astrophysical objects such as stellar interiors and atmospheres and protoplanetary disks.

Turbulent fluid flow contains a complex set of interacting submotions, or "eddies," which can be characterized by their individual sizes and kinetic energies. In typical turbulent flows, these sizes and energies span a wide range of values, the ranges being larger for flows of larger Reynolds number. Simulations of turbulent flow therefore become increasingly expensive for increasing Reynolds number and at some point are no longer feasible on available computers. To proceed, one must adopt approximations, or models, of some parts of the fluid motion, so that the remaining flow features can still be simulated at reasonable cost. The modeled motions are normally those of smallest size, and simulations incorporating such models are called large-eddy simulations. The missing, modeled eddies are referred to as unresolved.

The models of the small eddies, which are called sub-grid-scale models, incorporate dimensional and plausible-physics arguments to express the effect of these eddies on those still resolved. Typically, a dimensionless parameter is left to be fitted from experimental data or simulation results. Reasonable accuracy is obtained as long as the parameter-fitting and simulated flows are similar, or if "dynamic" models, which determine the free parameter "on-the-fly" based on current local flow conditions, are used; however, some flow types and features are not simulated well with these methods.

The flawed assumption in these models is that even the smallest eddies should have some perceptible, viscous-like effect on all other eddies. The models currently used in large-eddy simulations contain this effect implicitly, and this has been considered a correct modeling of the exact physics. However, recent very large-scale simulations have shown, on the contrary, that small eddies have essentially no direct effect on much larger ones: their effects are felt only indirectly through those of intermediate size.

Researchers at Stanford University and Ames Research Center have developed and tested a "multiscale" large-eddy simulation technique, which consists of applying the small-eddy model only to those eddies near in size to the unresolved ones, but including full interaction between these directly affected eddies and all others. Dramatically improved results are obtained both for fixed and dynamic model types. Figure 1 shows a comparison between a 256^3 direct numerical simulation of decaying isotropic turbulence and three 64^3 large-eddy simulations. The quantity being compared is the kinetic energy dissipation rate for all eddies resolved by a 64^3 grid, as a function of time; this quantity is particularly sensitive to the

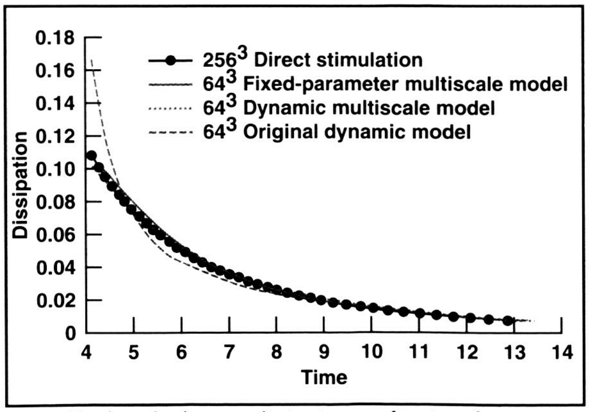

Fig. 1. Total resolved energy dissipation as a function of time, comparing three models with a direct numerical simulation.

accuracy of the simulation of the small-scale motions. It is clear that the dissipation rate is more accurately captured by the fixed-parameter multiscale model than by the original (non-multiscale) dynamic model, and that the dynamic multiscale model provides yet a further improvement in accuracy. The large initial error in the value as computed by the original dynamic model is quickly adjusted for by an overly large dissipation of the smallest resolved eddies, which reduces the dissipation rate to more nearly correct values at the cost of less accurate simulation of those eddies. The multiscale models do not suffer from this large initial error and do not apply excessive dissipation to the small eddies. Later, as the flow evolves, the small eddies decay away, lessening the need for sub-grid-scale modeling; as a result, all methods become quite accurate.

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Unstructured Large-Eddy Simulation Code for Simulation of Reacting Flows in Complex Geometries

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A large-eddy simulation (LES) unstructured mesh code for high-fidelity simulation of turbulent reacting flows has been developed. The code is designed to run on massively parallel supercomputers. It can handle complex geometries and is being used to compute the flow and associated combustion phenomena in an industrial gas turbine combustor in collaboration with Pratt and Whitney (P&W). LES is chosen because of its demonstrated superiority in predicting turbulent mixing over Reynolds-averaged Navier-Stokes (RANS) formulation. Accurate simulations of chemically reacting flows are critically dependent on the ability to accurately simulate turbulent mixing.

The numerical algorithm allows for the use of hybrid grids. It is a conservative non-dissipative formulation—second-order accurate on uniform grids. The energy-conserving properties of the algorithm allow us to obtain a robust method without the need to introduce numerical dissipation, as is generally done in RANS codes. Keeping the numerical dissipation at very low levels is essential to maintaining the accuracy of LES simulations. The code solves the incompressible flow equations or the low-Mach-number variable-density equations, the latter being used in simulations of reacting flows.

The dynamic LES model developed at the Center for Turbulence Research (CTR) is used to represent the subgrid stresses. The dynamic formulation offers many advantages when used in unstructured grid formulations, including dynamically computing the model coefficient (no empirical constants), eliminating the need for damping functions near solid surfaces, and eliminating the need for computing the distance to the wall.

Considerable effort was devoted to making the design of the code efficient. The code is fully parallel and uses Message Passing Interface. A novel algorithm was developed for grid-ordering, with the aim of minimizing processsor-to-processor communication. The code was ported to several platforms (e.g., Origin2000, IBM SP2, ASCI RED-Intel) and was